

On entropy, specific heat, susceptibility and Rushbrooke inequality in percolation

M. K. Hassan, D. Alam, M. Z. Islam and M. M. Rahman

University of Dhaka, Department of Physics, Theoretical Physics Group, Dhaka-1000, Bangladesh.

We investigate percolation, a paradigmatic model for continuous phase transition, on square and on weighted planar stochastic lattices. In its thermal counterpart, the critical exponents α , β and γ of specific heat, order parameter and susceptibility respectively are found to obey the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$. In percolation, however, it still remains elusive. In pursuit of this, we first investigate Shannon entropy and find that it undergoes a sharp drop near p_c revealing an order-disorder transition since Shannon entropy is a measure of information disorder or uncertainty. We then propose specific heat and susceptibility for percolation and find the corresponding critical exponents numerically. Finally, we show that the Rushbrooke inequality is obeyed for both the lattices albeit they belong to two different universality classes.

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The emergence of a well-defined critical value accompanied by a dramatic change in the properties of some physical quantities is always an indication of phase transition which we find in many seemingly disparate systems [1]. The study of phase transitions and critical phenomena have acquired a central focus in condensed matter and statistical physics due to their importance in science and technology. In general, phase transitions are classified into two classes depending on how an order parameter (OP), which is zero in one phase and non-zero in the other, varies below, at and above the critical point. In the first order phase transition, it suffers a jump or discontinuity at T_c and in the second order or continuous phase transition (CPT) it is continuous across T_c . The numerical value of OP in the CPT, which quantifies the degree of order, rises in the vicinity of T_c following a power-law OP $\sim \epsilon^\beta$ where $\epsilon \sim T - T_c$ is the distance from the critical point. The CPT is also characterized by the power-law growth of correlation length $\xi \sim \epsilon^{-\nu}$, specific heat $C \sim \epsilon^{-\alpha}$ and susceptibility $\chi \sim \epsilon^{-\gamma}$ in the vicinity of T_c and by their divergences at T_c . Remarkably, the numerical values of the critical exponents $\alpha, \beta, \gamma, \nu$ etc. are universal, in the sense that they depend only on the dimension of the systems and the range of interactions, and above all they are bound by some scaling relations. One of the most interesting scaling relations is the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$ which reduces to equality under static scaling hypothesis [1]. Many experiments and exactly solvable models too suggest that the Rushbrooke inequality actually holds as an equality [2].

Percolation is one of the simplest paradigmatic model for phase transition. To define it, one has to first choose a lattice. Then, each bond of the lattice is occupied randomly with probability p independent of the state of its neighbors [3, 4]. At p close to zero, the sites are mostly isolated or form small clusters where a cluster is a group of sites connected by occupied bonds. However, by tuning p further, one finds an intermediate p_c at which there appears a cluster for the first time that spans across the entire system. Such transition from isolated clusters to spanning cluster across p_c is found to be reminiscent of

the CPT. It is thus expected that for every observable quantity in the thermal CPT there should exist an equivalent counterpart in the percolation model too. In pursuit of this, Kasteleyn and Fortuin argued that the percolation strength $P(p)$, the ratio of the largest cluster to the lattice size $P = s_{\max}/N$, is like OP and the mean cluster size is like susceptibility [5, 6]. Recently, some authors have proposed the amplitude of the fluctuations of the $P(p)$ as a susceptibility [7–10]. Remarkably, like its thermal counterpart, percolation can also be classified into universality classes as we find that the critical exponents depend only on the dimensions of the lattice and on the types of percolation. Only recently there have been two exceptions to this, one in two dimensions [11] and the other in three dimensions [12, 13].

Despite nearly 60 years of extensive research, there are still some unresolved issues in percolation. First, we do not yet know how to define entropy albeit the association of disorder with percolation is as old as the model itself. Besides, an exact analogy of percolation with thermal CPT is only possible if we can show that the entropy undergoes a dramatic change across p_c such that it is large in one phase and negligibly small in the other. This would lead to conclude that percolation too is accompanied by order-disorder transition like ferromagnetic transition. A proper definition of entropy in percolation is thus long overdue. Second, we still do not know the equivalent counterpart of the specific heat, although it is one of the key parameters for CPT. Third, although we do not know the equivalent counterpart of specific heat, we still claim to know its critical exponent $\alpha = -2/3$ for regular planar lattice. This is obtained using Rushbrooke equality while taking for granted that equality holds in percolation. Finally, proving whether the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$ holds in percolation or not, remains elusive.

In this letter, we investigate bond percolation on two different planar lattices, namely square and weighted planar stochastic (WPS) lattices as skeleton, which belong to two different universality classes [11]. The details of the construction process of the WPS lattice and its properties can be found in Refs. [14–16]. First, we propose a suitable set of probabilities for Shannon entropy and

show that, like ferromagnetic transition, percolation is also an order-disorder transition. Second, we propose an exact equivalent counterpart of specific heat and susceptibility in analogy with their definition in its thermal counterpart. Then we use the finite-size scaling hypothesis to obtain the corresponding critical exponents and show once again that the two planar lattices belong to two distinct universality classes. Finally, and most importantly, we show that the elusive Rushbrooke inequality holds in both the lattices albeit they belong to two different universality classes.

To study percolation, we use the Newman-Ziff (NZ) algorithm which, apart from being the most efficient one, has also many other advantages [17]. For instance, it helps calculating various observable quantities over the entire range of p in every realization instead of measuring them for a fixed probability p in each realization. According to the NZ algorithm, all the labelled bonds $i = 1, 2, 3, \dots, M$ are first randomized and then arranged in the order in which they will be occupied. Note that the number of bonds with periodic boundary condition is $M = 2L^2$ for square lattice and $M \sim 8t$ for WPS lattice where t is the time step. In this way we can create percolation states consisting of $n+1$ occupied bonds simply by occupying one more bond to its immediate past state consisting of n occupied bonds. Initially, there are $N = L^2$ and $N = 3t + 1$ clusters of size one in the square and WPS lattices respectively. Occupying the first bond means forming a cluster of size two. Each time thereafter, either the size of an existing cluster grows due to occupation of inter-cluster bond or the cluster size remains the same due to occupation of intra-cluster bond. We calculate an observable, say X_n , as a function of n and use it in the convolution relation

$$X(p) = \sum_{n=1}^N p^n (1-p)^{N-n} X_n, \quad (1)$$

to obtain X as a function of p . The appropriate weight factor for each n at a given p is $\sum_{n=1}^N p^n (1-p)^{N-n}$. The convolution relation takes care of that weight factor and hence helps obtaining a smooth curve for $X(p)$.

The concept of cluster is central to the theory of percolation. Consider that for a given p there are m distinct, disjoint, and indivisible labelled clusters $i = 1, 2, \dots, m$ of size s_1, s_2, \dots, s_m respectively. It is then pretty straightforward to define $\mu_i(p) = s_i / \sum_{j=1}^m s_j$ as the probability that a site picked at random belongs to cluster i which is naturally normalized $\sum_{i=1}^m \mu_i(p) = 1$. The appropriate quantity to measure the uncertainty associated with the probabilities μ_i is the Shannon entropy

$$H = -K \sum_i^m \mu_i \log \mu_i, \quad (2)$$

where $K = 1/\log b$ and in information theory it is a common practice to assume $b = 2$ [18]. We will, however, set $K = 1$ since it merely amounts to a choice of a unit of

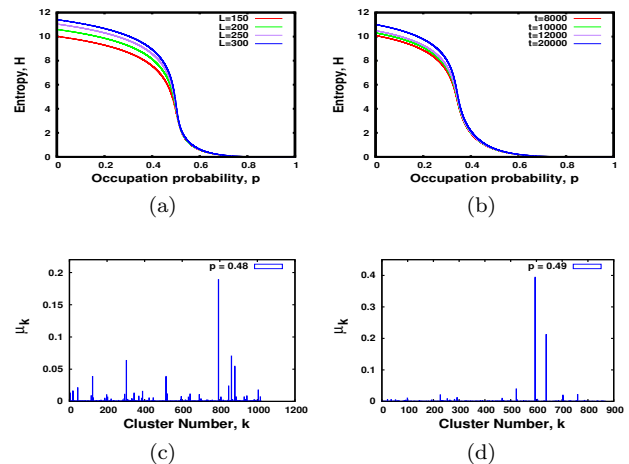


FIG. 1: Entropy H versus p for (a) square and (b) WPS lattice whose p_c values are 0.5 and 0.3457 respectively. Plots of μ_k vs k are shown only for square lattice at (c) $p = 0.48$ and (d) $p = 0.49$ just to illustrate how quickly μ changes as p approaches p_c .

measure of entropy. For a given distribution of cluster sizes the Shannon entropy measures how much information we need to locate a particular cluster in the system. In general, gaining information means making a displacement from the state of not knowing (uncertainty or confusion) to the state of knowing. In Figs. 1a and 1b, we plot entropy H as a function of p for both the lattices. We find that initially the entropy is maximum $H = \log(N)$ since at $p = 0$ each site is a cluster of size one and each cluster contributes in equal measure $\mu_i = 1/N$ to the information stored in H . This is exactly like the state of the isolated ideal gas which also corresponds to the maximum entropy and the most disordered state. We know that in the thermal CPT, the high temperature phase is almost always more disordered (high entropy) than the low temperature phase. In percolation, the driving parameter is p and $1-p$ is the equivalent counterpart of temperature. Thus according to Figs. 1a and 1b, we can say that the high $1-p$ phase is more disordered than the low $1-p$ phase if we regard uncertainty or confusion, which is measured by H , as an equivalent counterpart of disorder.

To understand what happens in the vicinity of p_c , we give two representative plots of μ_k vs k in Figs. 1c and 1d for $p = 0.48, 0.49$ respectively. It clearly reveals that near p_c , even an infinitesimal change in p causes significant change in the distribution of μ_k . This is due to the fact that in the vicinity of p_c , the coagulation of two clusters takes place more frequently than the formation of isolated clusters of single site or growth of existing cluster by one unit due to agglomeration. Finally, at and above p_c , the incipient spanning cluster is so prevailing that if we pick an occupied site at random it will most likely be a part of the spanning cluster. As p increases further, the extent of this uncertainty diminishes $H \rightarrow 0$

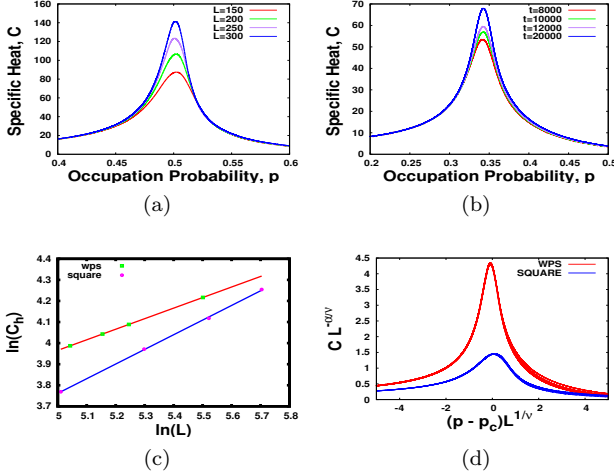


FIG. 2: Specific heat $C(p)$ vs p for (a) square and (b) WPS lattices. In (c) we plot $\log(C_h)$ versus $\log(L)$ and find $\alpha/\nu = 0.68(1)$ and $\alpha/\nu = 0.5007(3)$ for square and WPS lattices respectively. (d) Plots of $C(p)L^{-\alpha/\nu}$ vs $(p-p_c)L^{1/\nu}$ for square and WPS lattices and find that all the distinct plots in (a) and (b) collapse into their respective universal curves.

as p increases beyond p_c . However, at and around p_c the extent of uncertainty, which is the equivalent counterpart of disorder, drops sharply revealing that percolation too is an order-disorder transition. Thus, we can say that the order parameter $P = 0$ corresponds to more disordered phase than the phase where $P > 0$ which is clearly reminiscent of the ferromagnetic transition.

To find an equivalent counterpart of the specific heat in percolation we find it worthwhile first to consider its thermodynamic definition $C = T \frac{dS}{dT}$ where S is the thermodynamic entropy [1]. In analogy with this, we can define it for percolation as

$$C(p) = (1-p) \frac{dH}{d(1-p)}, \quad (3)$$

where S has simply been replaced by Shannon entropy H and T by $1-p$. To check what happens to $C(p)$ we plot it in Figs. 2a and 2b for both square and WPS lattices as a function of p for different system size. We observe that, for a given system size, the peak always occurs almost at p_c and the peak value increases quite sharply with system size L and decreases above p_c without having to exclude the spanning cluster. We can write the finite-size scaling (FSS) hypothesis

$$C(p, L) \sim L^{\alpha/\nu} \phi_C((p-p_c)L^{1/\nu}), \quad (4)$$

where ϕ_C is the scaling function for specific heat. It implies that the two quantities $CL^{-\alpha/\nu}$ and $(p-p_c)L^{1/\nu}$ are dimensionless and hence all the distinct plots of C vs p should collapse onto a single universal curve ϕ_C if we plot $C/L^{-\alpha/\nu}$ vs $(p-p_c)L^{1/\nu}$. To find an estimate for the exponent α/ν , we measure the height of the peak C_h at

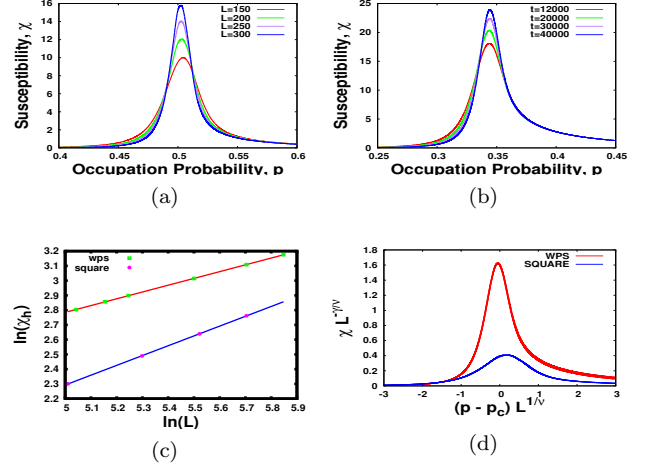


FIG. 3: Plots of χ vs p for (a) square and (b) WPS lattice. In (c) we plot $\log(\chi_h)$ vs $\log(L)$ and find that $\gamma/\nu = 0.635(2)$ and $\gamma/\nu = 0.460(1)$ for square and WPS lattices respectively. In (d) we plot $\chi L^{-\gamma/\nu}$ vs $(p-p_c)L^{1/\nu}$ and find that all the distinct plots in (a) and (b) collapse into their respective universal curves.

p_c as a function of L . Plotting $\log(C_h)$ versus $\log(L)$ we get straight lines, see Fig. 2c, with slopes $\alpha/\nu = 0.68(1)$ for square lattice and $\alpha/\nu = 0.5007(3)$ for WPS lattice. If we now plot $CL^{-\alpha/\nu}$ as a function of $(p-p_c)L^{1/\nu}$ then we find that all the distinct plots for both cases of Figs. 2a and Figs. 2b collapse into their own universal curve as they belong to the separate universality classes (see Fig. 2d). Using the relation $L \sim (p-p_c)^{-\nu}$ in $C(p) \sim L^{\alpha/\nu}$ we can immediately find that the specific heat diverges

$$C(p) \sim (p-p_c)^{-\alpha}, \quad (5)$$

with $\alpha = 0.906(13)$ for square lattice and $\alpha = 0.816(4)$ for WPS lattice.

To find an equivalent counterpart of susceptibility in percolation we focus on the change in the ΔP within an interval $\Delta p = \frac{1}{M}$ where $M = 2L^2$ bonds for square lattice and $M \sim 8t$ bonds for WPS lattice. It is done by keeping track of the increase or jump in $P = s_{\max}/N$ each time we occupy a bond. The successive jump in OP therefore is $\Delta P = \Delta s_{\max}/N$ and hence we can define the susceptibility as $\chi(p) = \frac{\Delta P}{\Delta p}$. It essentially describes the derivative of P with respect to p since $\Delta p \rightarrow 0$ in the large N limit. Note that susceptibility is a response function which is indeed the first derivative of the OP. In Figs. (3a) and (3b) we plot $\chi(p)$ as a function of p for both types of lattice and find that $\chi(p)$ grows as we increase p and as we approach p_c the growth is quite steep. However, beyond p_c it decreases sharply without excluding the size of the spanning cluster. This is in sharp contrast to the existing definition of susceptibility, which is the mean cluster size as it strictly requires exclusion of the spanning cluster. To find the exponent γ , we apply

the FSS hypothesis

$$\chi(p, L) \sim L^{\gamma/\nu} \phi_\chi((p - p_c)/L^{-1/\nu}), \quad (6)$$

where ϕ_χ is the scaling function for susceptibility. Following the same procedure done for $C(p)$, we find $\gamma/\nu = 0.635(2)$ for square lattice and $\gamma/\nu = 0.460(1)$ for WPS lattice. If we now plot $\chi L^{-\gamma/\nu}$ versus $(p - p_c)L^{1/\nu}$ then we find that all the distinct plots of Figs. 3a and 3b collapse into their own distinct universal curve as shown in Fig. 3d. It implies that

$$\chi(p) \sim (p - p_c)^{-\gamma}, \quad (7)$$

where $\gamma = 0.846(2)$ and $\gamma = 0.750(6)$ for square and WPS lattices respectively.

Lattice	α	β	γ	$\alpha + 2\beta + \gamma$
Square	0.906	0.1388	0.846	2.029
WPS	0.816	0.222	0.750	2.01

TABLE I: The critical exponents and Rushbrooke inequality for square and WPS lattice.

Scaling theory predicts that the various critical exponents cannot just assume values independently rather they are bound by some scaling relations. One of the relations is the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$. Remarkably, many experiments and exactly solved models of thermal CPT suggest that it is the Rushbrooke equality that holds more often than its inequality. The static Widom scaling (SWS), which is based on the simple assumption that the Gibbs free energy is a generalized homogeneous function, also suggests such equality

[1]. Substituting α , γ and β for square and WPS lattices we find that the Rushbrooke inequality, rather equality within the limits of error, holds in percolation (see table I).

To summarize, in this article we proposed the equivalent counterpart of entropy, specific heat and susceptibility for percolation model. The introduction of the Shannon entropy helped appreciating the fact that like thermal CPT, percolation too is accompanied by order-disorder transition across p_c . However, in percolation disorder means information disorder or uncertainty quantified by high H and order corresponds to low entropy that describes the state of less missing information or less uncertainty. This analogy helps to conclude that, like in ferromagnetic transition, the OP in percolation is zero in the disordered phase and non-zero in the ordered phase. We then showed that the specific heat and susceptibility both exhibit divergence at p_c following power-law near p_c without having to exclude the spanning cluster from their calculation. Using the FSS hypothesis and the idea of data-collapse, we numerically obtained the critical exponents α and γ for both square and WPS lattices. We find that their values in the two lattices do not coincide which once again confirms that they belong to two different universality classes. Finally, we showed that the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$, which is more equality than inequality, holds in percolation on both the lattices albeit they belong to two distinct universality classes. The new idea of entropy, specific heat and susceptibility will definitely have far reaching impacts in making percolation a truly paradigmatic model for continuous phase transition.

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